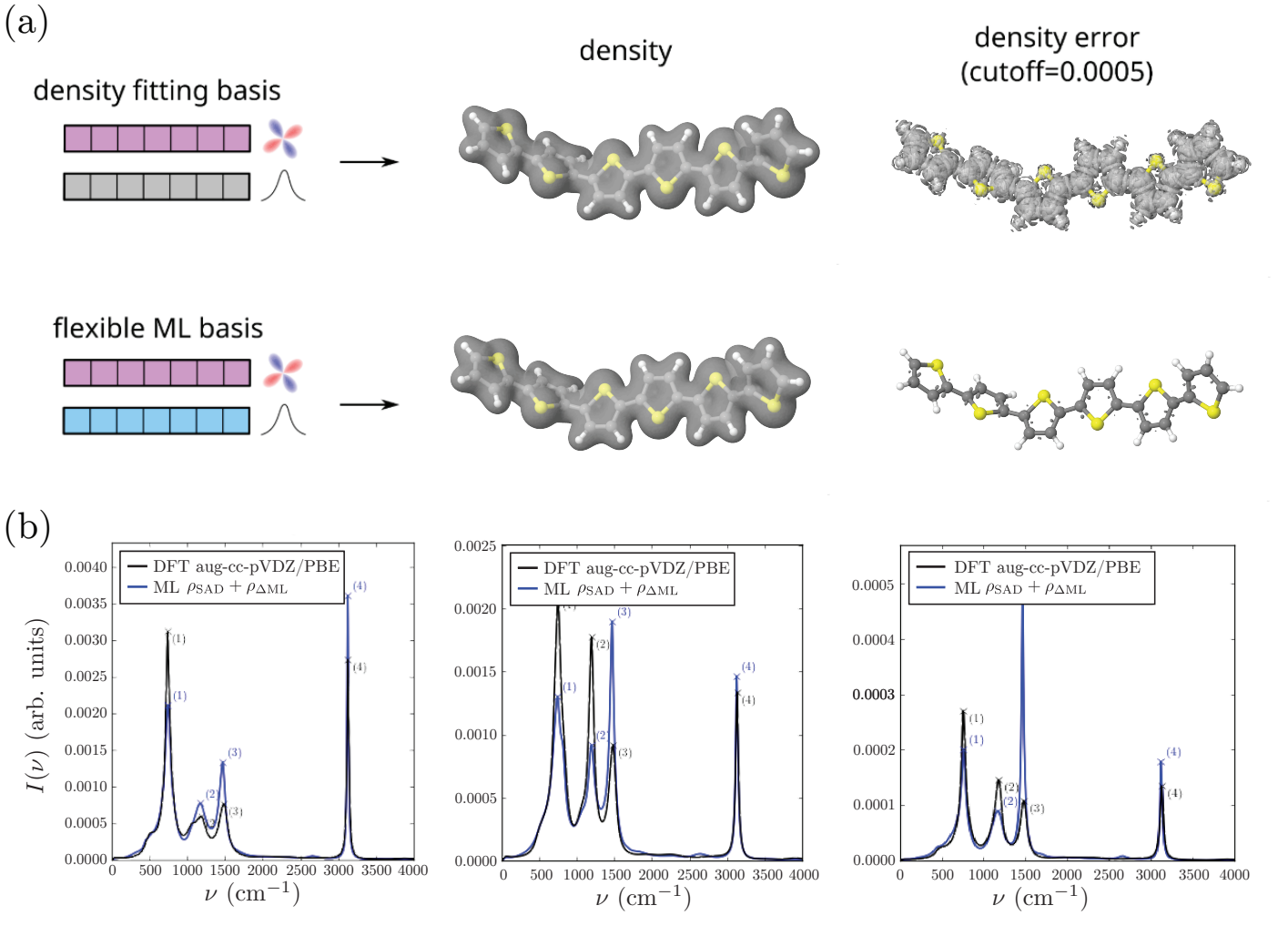

(a)
density fitting basis
density
density error
(cutoff=0.0005)
flexible ML basis
(b)
DFT aug-cc-pVDZ/PBE
ML $\rho_{\mathrm{SAD}} + \rho_{\Delta\mathrm{ML}}$
$I(\nu)$ (arb. units)
ν (cm^{-1})